Multichannel Schwinger variational cross sections for electron-impact excitation of the $b\ ^3\Sigma_u^+$ state in H_2

Marco A. P. Lima,* Thomas L. Gibson, Kazuo Takatsuka,† and Vincent McKoy
Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125
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As a first application of the Schwinger multichannel theory, we have calculated integral and differential cross sections for electron-impact excitation of the transition $X\ ^1\Sigma_g^+ \rightarrow b\ ^3\Sigma_u^+$ in H_2 for scattering energies from 13 to 30 eV at the two-state level. We find good agreement between our integral cross sections and the results obtained previously in a two-state close-coupling study. Our method does not rely on single-center expansions to calculate the body-frame scattering amplitude and is designed to be applicable to molecules of arbitrary geometry.

I. INTRODUCTION

Accurate cross sections for the electronic excitation of molecules by low-energy ($\lesssim 30$ eV) electron impact are important for a variety of reasons. Measurements[1] in this energy region can often be difficult and time consuming, and hence theoretical studies of these cross sections for linear and small polyatomic targets are obviously desirable. In particular, the differential cross sections give considerable insight into the physics of the electron-molecule interaction as well as providing a sensitive test of the collision theory being used. This last point is quite important since a number of theoretical approaches involving varying degrees of approximation are available. These approaches include plane-wave theories such as the Born-Ochkur-Rudge approximations,[2,3] the impact-parameter method,[4] distorted-wave theories,[5,6] and multichannel theories. Plane-wave theories are lowest-order theories containing approximations valid at high impact energies. These theories are computationally easy to apply, but recent studies[7,8] have shown that they lead to qualitatively and quantitatively incorrect differential cross sections at low and intermediate electron energies. The impact-parameter method[4] is a semiclassical approach in which the projectile electron is treated classically and although this method can provide some improvement over plane-wave theories, it does not include enough of the collision physics to produce reliable differential cross sections at low energies. A distorted-wave approach is the next logical step beyond the plane-wave theories. Recently, studies using a distorted-wave approximation[7,8] in the 20–100 eV range have shown that this method can predict differential cross sections in qualitative agreement with measured values. However, there are serious quantitative disagreements between these distorted-wave cross sections and available data in several cases.[8] Multichannel theories of these inelastic collisions have the firmest theoretical basis, but they are considerably more difficult to apply. However, at the two-state level of approximation, close-coupling calculations for selected transitions in H_2 have been carried out by Chung and Lin[9] and by Weatherford[10] and for the $a\ ^1\Pi_g$ channel in N_2 by Holley *et al.*[11] Both Chung and Lin and Weatherford obtained integral cross sections for the exchange-allowed excitation $X^1\Sigma_g \rightarrow b^3\Sigma_u^+$, but only Weatherford reports differential cross sections for this channel.

In this paper we report the first results[12] obtained from the application of a Schwinger multichannel (SMC) formulation to electronically inelastic electron-molecule collisions. Specifically, we have calculated integral and differential cross sections for the $X^1\Sigma_g^+ \rightarrow b^3\Sigma_u^+$ excitation in H_2 for impact energies from 13 to 30 eV. Some formal details of our method are discussed in an accompanying paper.[13] An important feature of this formulation is that it can provide an analytic approximation to the multichannel scattering amplitude in the plane-wave representation, thereby obviating the need for single-center expansions. As a consequence of this feature, our method has been designed to be applicable to molecules of *arbitrary* geometry and to include a significant number of open and closed electronic channels.

In Sec. II we present a brief review of the SMC formulation. The computational details of our study can be found in Sec. III together with a discussion of our results and a comparison with other studies. In Sec. IV we summarize our findings and conclusions.

II. THEORY

The details of the SMC formalism have been presented in a companion paper,[13] and hence we will give only a brief review here. Our method begins with a projected Lippman-Schwinger equation

$$P\Psi_n^{(+)} = \frac{1}{\sqrt{N+1}} S_n + G_P^{(+)} V \Psi_n^{(+)} , \tag{2.1}$$

where $\Psi_n^{(+)}$ is the total $(N+1)$-particle wave function with plane-wave and outgoing-wave boundary conditions for the nth channel. The projection operator P defines the open-channel space in terms of eigenfunctions of the target Hamiltonian H_N

$$P = \sum_{m=1}^{N_0} |\Phi_m(1,2,\ldots,N)\rangle\langle\Phi_m(1,2,\ldots,N)| \tag{2.2}$$

and

$$H_N|\Phi_m\rangle=E_m|\Phi_m\rangle,\quad E-E_m>0 \tag{2.3}$$

where E is the total energy of the $(N+1)$-particle system. In Eq. (2.1) S_n is the free-particle solution of the unperturbed Hamiltonian $H_0=H_N+T_{N+1}$ and is given by

$$S_n=\Phi_n e^{i\vec{k}_n\cdot\vec{r}_{N+1}}. \tag{2.4}$$

The interaction potential V is

$$V=H_{N+1}-H_0=\sum_{i=1}^{N}\frac{1}{|\vec{r}_i-\vec{r}_{N+1}|}-\sum_{\alpha}\frac{Z_\alpha}{|\vec{R}_\alpha-\vec{r}_{N+1}|}, \tag{2.5}$$

where the first term on the right-hand side (rhs) of Eq. (2.5) represents the interaction between the incident and target electrons and the second term represents the interaction between the incident electron and the nuclei. The outgoing-wave Green's function $G_P^{(+)}$, which is defined only in the *open*-channel space, can be written as

$$G_P^{(+)}=\sum_{m=1}^{N_0}|\Phi_m\rangle g_m^{(+)}(\vec{r}_{N+1},\vec{r}\,'_{N+1})\langle\Phi_m| \tag{2.6}$$

with

$$g_m^{(+)}(\vec{r},\vec{r}\,')=-\frac{1}{2\pi}\frac{e^{ik_m|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}. \tag{2.7}$$

As shown by Takatsuka and McKoy,[12,13] a complete equation for $\Psi_n^{(+)}$ is given by

$$\left[\frac{1}{2}(PV+VP)-VG_P^{(+)}V+\frac{1}{N+1}\left[\hat{H}-\frac{N+1}{2}(P\hat{H}+\hat{H}P)\right]\right]\Psi_n^{(+)}=\frac{1}{\sqrt{N+1}}VS_n, \tag{2.8}$$

where $\hat{H}=E-H_{N+1}$. This equation contains information about the closed electronic channels without defining the *closed*-channel Green's function which would necessitate including the target continuum states.[14] Based on Eq. (2.8), a variational functional for the fixed-nuclei scattering amplitude is

$$f^B(\vec{k}_m,\vec{k}_n)=-\frac{1}{2\pi}\frac{\langle S_m|V|\Psi_n^{(+)}\rangle\langle\Psi_m^{(-)}|V|S_n\rangle}{\left\langle\Psi_m^{(-)}\left|\left[\frac{1}{2}(PV+VP)-VG_P^{(+)}V+\frac{1}{N+1}\left[\hat{H}-\frac{N+1}{2}(P\hat{H}+\hat{H}P)\right]\right]\right|\Psi_n^{(+)}\right\rangle}, \tag{2.9}$$

where the superscript B on f^B indicates that this quantity is calculated in the body-fixed (molecular) reference frame.[15]

In our procedure $\Psi_n^{(+)}$ is expanded in a basis of Slater determinants which are constructed from an orthogonal set of molecular orbitals, additional basis functions, and plane-wave functions, if necessary. These molecular orbitals and additional basis functions are further expanded in Cartesian Gaussian functions. With this choice of basis all of the matrix elements appearing in Eq. (2.9), except for the matrix elements of $VG_P^{(+)}V$, can be evaluated analytically. However, these matrix elements can also be obtained in closed form[16–18] if an approximate closure relation is inserted around $G_P^{(+)}$, viz.,

$$\langle\Psi_m^{(-)}|VG_P^{(+)}V|\Psi_n^{(+)}\rangle\cong\sum_{\substack{\gamma,\gamma'\\ \delta,\delta'}}\langle\Psi_m^{(-)}|V|\gamma\rangle(\underline{Q}^{-1})_{\gamma,\gamma'}\times\langle\gamma'|G_p^{(+)}|\delta\rangle(\underline{Q}^{-1})_{\delta,\delta'}\langle\delta'|V|\Psi_n^{(+)}\rangle, \tag{2.10}$$

where $(\underline{Q})_{\gamma,\gamma'}=\langle\gamma|\gamma'\rangle$ and Cartesian Gaussian functions are again chosen for the insertion basis $|\gamma\rangle$. This insertion basis can be larger than the one used to expand $\Psi_n^{(+)}$. The form of the insertion used in Eq. (2.10) does not require that $|\gamma\rangle$ be an orthonormal set. Thus, we can include the SCF orbitals, additional scattering functions, and extra Gaussians used only for insertion to make up the $|\gamma\rangle$ basis. A criterion for the completeness of this insertion basis can be obtained by observing the way in which the scattering matrix approaches unitarity.

This formulation allows us to obtain an analytic approximation to the body-frame fixed-nuclei[15,19,20] scattering amplitude f^B for molecules of arbitrary geometry. To generate the physical differential cross section, one needs the laboratory-frame[15] scattering amplitude f^L. As a first step to acquiring this quantity we expand f^B in a partial-wave series

$$f^B(\vec{k}_m,\vec{k}_n)=\sum_{l,\bar{m}}F^B_{l,\bar{m}}(k_m,\vec{k}_n)Y_l^{\bar{m}}(\hat{k}_m). \tag{2.11}$$

Here, $F^B_{l,\bar{m}}$ is given by

$$F^B_{l,\bar{m}}(k_m,\vec{k}_n)=\int d\hat{k}_m\,Y_l^{\bar{m}}(\hat{k}_m)^*f^B(\vec{k}_m,\vec{k}_n). \tag{2.12}$$

An N-point Gauss-Legendre quadrature is used to perform each of the angular integrations in Eq. (2.12); for given k_m and k_n this requires that $f^B(\vec{k}_m,\vec{k}_n)$ be determined at the appropriate set of angles. A straightforward application of the Wigner rotation matrices[21] is then used to obtain f^L as a partial-wave series expanded in terms of the laboratory-frame angles $\hat{k}'_m$, viz.,

$$f^L(\vec{k}'_m,\vec{k}_n)=\sum_{l,\bar{m},\bar{\mu}}F^B_{l,\bar{m}}(k_m,\vec{k}_n)Y_l^{\bar{\mu}}(\hat{k}'_m)D^l_{\bar{\mu}\bar{m}}(0,\beta,\alpha), \tag{2.13}$$

where $\vec{D}$ is the rotation matrix whose argument consists of the Euler angles relating the two reference frames. The random orientation of the target is accounted for by explicitly averaging over the angles $\hat{k}_n$. If the laboratory-frame angles $\hat{k}'_m$ are denoted by (θ',ϕ'), the differential cross section can be written as

$$\sigma(\theta',\phi';k_m,k_n)=\frac{1}{4\pi}\frac{k_m}{k_n}\int d\hat{k}_n\,|f^L(\vec{k}'_m,\vec{k}_n)|^2 . \quad (2.14)$$

Again, Gauss-Legendre quadratures are used to perform the angular integrations. Finally, the physical cross section is obtained by averaging over the azimuthal angle ϕ' and performing the appropriate average over initial and sum over final spin states for the transition of interest.

III. PROCEDURE AND RESULTS

As a first application of our formulation we have obtained the differential and integral cross sections for excitation of the $b^3\Sigma_u^+$ state of H_2 by 13–30 eV electrons. This excitation is a very convenient example for our present purpose since it is one of the very few molecular systems that have been studied by close-coupling techniques.[9,10] As in these close-coupling studies we include only two open channels and completely neglect any closed channels. Moreover, these cross sections have also been studied by plane-wave theories[2,3] and distorted-wave methods.[6,7]

Our calculations are performed within the framework of the fixed-nuclei and Franck-Condon approximations.[15,19,20] The rotational levels are treated as degenerate and the physical cross sections are obtained by averaging the fixed-nuclei results over all molecular orintations. A single electronic transition matrix element is calculated with outgoing electron energy determined by the vertical transition energy from the $v=0$ ground state to the final vibrational level with the largest Frank-Condon factor. The value of the threshold energy determined this way is taken to be 10.5 eV. Unless otherwise stated, atomic units are used throughout.

For the ground state we used a self-consistent-field (SCF) wave function obtained with a $(5s\,2z)^*$ Cartesian Gaussian basis at an internuclear distance of 1.4003 r_0. This basis has been used previously[22] and for convenience is shown in Table I. The SCF energy was $-1.132\,564$ a.u. For the $b^3\Sigma_u^+(1\sigma_g 1\sigma_u)$ state we make the frozen-core approximation and determine the $1\sigma_u$ orbital by diagonalizing the V_{N-1} potential of the core in the SCF bais. The vertical excitation energy for the $b^3\Sigma_u^+$ state in this basis set is 9.97 eV from the $v=0$ vibrational level. This entire set of V_{N-1} eigenfunctions, i.e., improved virtual orbitals (IVO),[23] is available for use in expanding the $(N+1)$-particle wave function. The Gaussian basis sets used as additional scattering functions and in the insertion basis are also shown in Table I. For this exchange exciation expansion of the scattering functions solely in discrete basis functions should be adequate.

In the body frame all calculated results include the Σ_g, Σ_u, Π_g, and Π_u symmetries of the $(N+1)$ particle functions $\Psi_m^{(\pm)}$. Of the available scattering basis, no more than 17 (10) spatial functions were used to construct the determinants included in the expansion of $\Psi_m^{(\pm)}$ for $\Sigma(\Pi)$ symmetries. For the Σ symmetries, the scattering set consits

TABLE I. Basis sets for these calculations.[a]

SCF[b]		$^2\Sigma_{g,u}^+$[c]		$^2\Pi_{g,u}$[d]		Extra insertion[e]	
			$A=(0,0,\pm 0.70014)$				
$l\ m\ n$	α			$l\ m\ n$	α	$l\ m\ n$	α
0 0 0	48.4479			1 0 0	1.08	0 0 0	0.086
0 0 0	7.28346			1 0 0	0.54	0 0 0	3.142
0 0 0	1.65139			1 0 0	0.18	0 0 1	3.0
0 0 0	0.462447			1 0 0	0.06	1 0 0	0.3118
0 0 0	0.145885			1 0 0	0.02	1 0 0	0.1039
0 0 1	1.5					1 0 0	0.0346
0 0 1	0.5					1 0 0	0.0115
		$A=(0,0,0)$					
		$l\ m\ n$	α			$l\ m\ n$	α
		0 0 0	1.0			0 0 0	2.0
		0 0 0	0.2			0 0 0	0.5
		0 0 0	0.1			0 0 0	0.05
		0 0 1	1.0			0 0 0	0.01
		0 0 1	0.2			0 0 1	2.0
						0 0 1	0.5
						0 0 1	0.1
						0 0 1	0.05
						0 0 1	0.01

[a]Cartesian Gaussian functions defined by $X_{lmn}^{(\alpha)}=N_{lmn}(x-A_x)^l(y-A_y)^m(z-A_z)^n e^{-\alpha|\vec{r}-\vec{A}|^2}$.

[b]Basis set used for the $X^1\Sigma_g^+(1\sigma_g)^2$ ground and $b^3\Sigma_u^+(1\sigma_g 1\sigma_u)$ excited states of H_2.

[c]Additional functions used to expand the scattering functions for $^2\Sigma_{g,u}^+$ symmetries.

[d]Same as c but for the $^2\Pi_{g,u}$ symmetries.

[e]Extra set of functions used in the insertion around $VG_P^{(+)}V$ [see Eq. (2.10)].

TABLE II. Differential cross sections for excitation of the $b^3\Sigma_u^+$ state (10^{-18} cm^2).

Scattering angle (deg)	Impact energy (eV) 13	15	20	25	30
0	3.48	4.41	4.19	2.73	1.90
10	3.41	4.33	4.18	2.77	1.95
20	3.22	4.10	4.11	2.86	2.05
30	2.91	3.70	3.92	2.90	2.11
40	2.50	3.16	3.57	2.81	2.05
50	2.05	2.53	3.03	2.50	1.82
60	1.59	1.88	2.34	2.01	1.44
70	1.20	1.32	1.60	1.42	0.997
80	0.946	0.958	0.977	0.860	0.594
90	0.879	0.896	0.602	0.465	0.322
100	1.02	1.18	0.571	0.319	0.230
110	1.37	1.79	0.896	0.437	0.300
120	1.87	2.65	1.51	0.767	0.482
130	2.46	3.63	2.28	1.22	0.711
140	3.07	4.60	3.06	1.69	0.930
150	3.61	5.44	3.74	2.10	1.10
160	4.03	6.09	4.24	2.40	1.22
170	4.30	6.48	4.54	2.59	1.29
180	4.39	6.61	4.64	2.65	1.31

of a mixture of IVO's and additional functions chosen to improve the flexibility of the basis. However, since there are no π orbitals in the IVO set, the scattering basis for the Π symmetries is made up entirely of additional scattering functions. As discussed in Sec. II, the insertion basis used to calculate the matrix elements of $VG_P^{(+)}V$ is larger than the SCF and scattering basis sets. The extra Gaussian functions used in the insertion basis and shown in Table I significantly improved the unitarity of the scattering matrix compared with the results obtained when only the SCF and scattering basis functions are used.

We used an 8-point Gauss-Legendre quadrature for the integration over θ in Eqs. (2.12) and (2.14) along with a 6-point quadrature for each "hemisphere" of the integration over ϕ. For a given k_m and k_n, this requires a 96 by 96 matrix of values for $f^B(\vec{k}_m,\vec{k}_n)$, many of which need not actually be computed since they are related by symmetry to other matrix elements. Also, for the scattering energies considered here, we restrict the partial-wave expansion of the inelastic scattering amplitude in Eq. (2.11) to values of $l \leq 3$.

Table II gives the inelastic differential cross sections for several incident energies. The $b^3\Sigma_u^+$ state is dissociative and hence all its vibrational states lie in the continuum. All our cross sections are those for the complete band system, i.e., summed over all final vibrational levels. At the lower incident energies in these studies this assumption is not quite correct since the sum of Franck-Condon factors for the "open" vibrational levels is still only about 0.9. However, for the present purposes it is convenient to report essentially the fixed-nuclei cross sections for

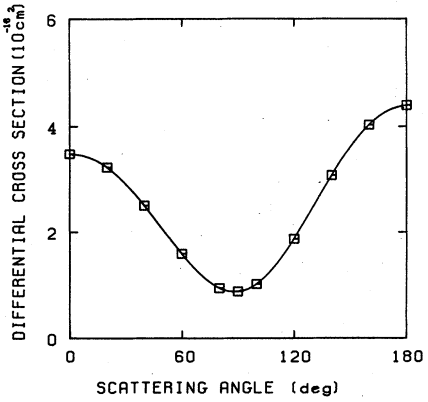

FIG. 1. Differential cross section (DCS) for excitation of the $b^3\Sigma_u^+$ state at 13 eV.

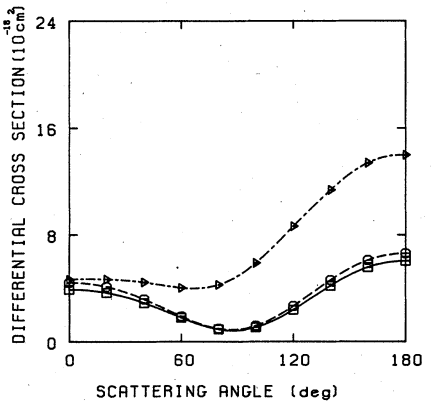

FIG. 2. DCS for excitation of the $b^3\Sigma_u^+$ state at 15 eV: present results with π-scattering functions on the center (——); results with π-scattering functions on the nuclei (— — —); distorted wave (DW) results of Ref. 7 (—·—·-).

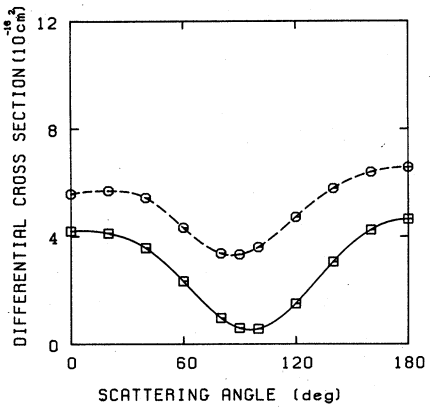

FIG. 3. DCS for excitation of the $b^3\Sigma_u^+$ state at 20 eV: present results (——); DW results of Ref. 7 (— — —).

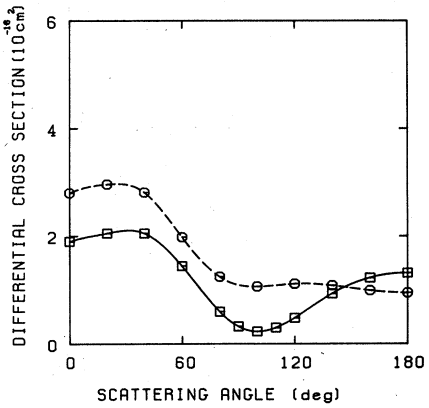

FIG. 5. DCS for excitation of the $b^3\Sigma_u^+$ state at 30 eV: present results (——); DW results of Ref. 7 (— — —).

$R = 1.4003a_0$ and we hence do so.

These differential cross sections are also shown in Figs. 1–5. The substantial backward peaking of these exchange-type excitation cross sections at the lower incident energies is very evident. In Figs. 2–5, we also show the differential cross sections at 15, 20, 25, and 30 eV obtained by Fliflet and McKoy[7] using a distorted-wave theory. At incident energies of 20, 25, and 30 eV the distorted-wave cross sections are in reasonable qualitative agreement with those of the present two-state calculations. This agreement is clearly better for scattering angles below 120°. However, Fig. 2 shows that for 15 eV the distorted-wave differential cross sections are in very poor agreement with the present results. This disagreement between the distorted-wave approximation and a two-state calculation at lower incident energies is not surprising. In Fig. 4 we also compare our differential cross sections with those of Weatherford's two-state calculation at 25 eV. In addition to their generally larger values the present cross sections do not fall off as rapidly in the forward direction as those of Weatherford.

In computing these results we found that contributions from the Π symmetry have considerable effect on the overall shape and magnitude of the differential cross sections. Thus in order to test the sensitivity of the scattering results to our choice of basis functions for the Π symmetry (see Table I), we performed an additional set of calculations using different Π basis functions located on the molecular center. Differential cross sections corresponding to a scattering energy of 15 eV are shown in Fig. 2 for the two sets of calculations. These results are in reasonable agreement with each other and, in fact, the agreement at higher energies (not shown) is even better.

Our corresponding integral cross sections for excitation of the $b^3\Sigma_u^+$ state are given in Table III along with Born-Rudge results,[2,9] the distorted-wave values of Fliflet and McKoy,[7] and the close-coupling results of Chung and Lin.[9] These cross sections are also shown in Fig. 6 where we see that the close-coupling cross sections of Chung and Lin are in good agreement with the present results. The close-coupling results of Weatherford[10] (not shown) differ somewhat from those of Chung and Lin;[9] they are smaller

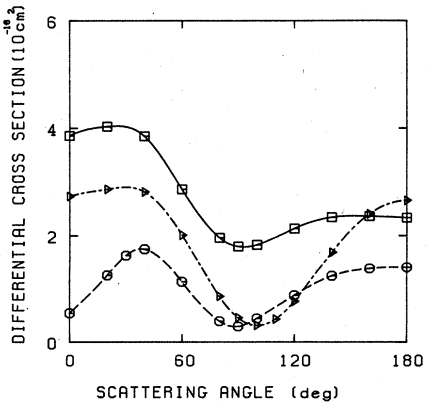

FIG. 4. DCS for excitation of the $b^3\Sigma_u^+$ state at 25 eV: present results (——); DW results of Ref. 7 (——); close-coupling (CC) results estimated from Fig. 6 of Ref. 10 (— — —).

TABLE III. Integral cross sections for excitation of the $b^3\Sigma_u^+$ state (10^{-17} cm^2).

Impact energy (eV)	DW[a]	BR[b]	CC[c]	SMC[d]
11.0	3.50			
12.0	6.25			
13.0	7.85	4.47	2.19	2.46
14.0		4.41	2.56	
15.0	8.30	4.18	2.80	3.25
16.0	8.03	3.88	2.84	3.28
17.5		3.41	2.81	
18.0	6.81			
20.0	5.78	2.69	2.53	2.69
22.0	4.53			
25.0	3.16	1.70	1.82	1.85
30.0	1.95	1.10	1.26	1.23

[a]Distorted wave results of Ref. 7.
[b]Born-Rudge results of Ref. 9.
[c]Two-state close-coupling results of Ref. 9.
[d]Present results.

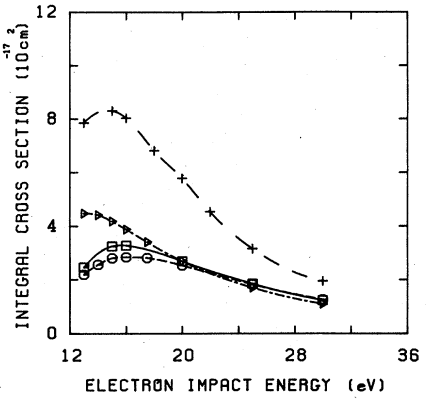

FIG. 6. Integral cross section for excitation of the $b^3\Sigma_u^+$ state: present results (——); CC results of Ref. 9 (— — —); Born-Rudge results of Ref. 9 (—·—·—); DW results of Ref. 7 (— — —).

and peak at about 3 eV lower in energy than those of Chung and Lin.[9] The distorted-wave theory clearly overestimates the integral cross section by about a factor of 2, although the shapes of the corresponding differential cross sections are in reasonable agreement with the SMC results. The Born-Rudge cross sections are somewhat larger and peak at lower energy than those of the other methods. We do not show a comparison with the measurements of Corrigan[24] since these data contain significant contributions from channels not included in the present study, and hence, these experimental cross sections are larger than the two-state SMC or close-coupling results for exciting only the $b^3\Sigma_u^+$ state.[9]

IV. CONCLUSIONS

In this paper we have reported the first application of a Schwinger multichannel formulation to low-energy electron-impact excitation of the $b^3\Sigma_u^+$ state of H_2. For consistency in comparing with other theoretical results, our cross sections were calculated at the two-state level and closed-channel effects were not included. No reliable experimental data are available for these cross sections. However, our integral cross sections agree quite well with the close-coupling results of Chung and Lin.[9] Although Chung and Lin do not report differential cross sections, a comparison at 20, 25, and 30 eV shows qualitative agreement between our differential cross sections and the distorted-wave values of Fliflet and McKoy.[7]

With the SMC formulation, our procedure allows us to compute an analytical approximation to the multichannel fixed-nuclei scattering amplitude without resorting to single-center expansions. As a result, our method is well suited for applications to molecules of arbitrary geometry and for inclusion of a substantial number of open and closed channels. The method can be applied straightforwardly to study low-energy electron collisions with a variety of small polyatomic targets. Calculations for e-N_2 and e-CH_4 scattering are underway.

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*Permanent address: Instituto de Estudos Avançados, Centro Técnico Aeroespacial, 12200 São José dos Campos, São Paulo, Brazil.

†Present address: Institute for Molecular Science, Myodaiji, Okazaki 444, Japan.

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